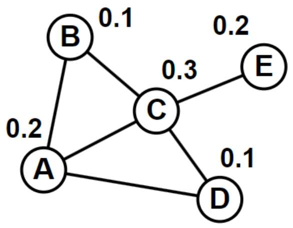
Final Exam (Graph Neural Networks –Fall 2023)

Full Name:
Student ID:

1. Consider an undirected graph G of five nodes A, B, C, D, and E given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $h_A^{(0)} = 0.2$). According to GraphSAGE model with a AGGREGATE is a MEAN function, the feature of a node i at layer k can be updated as:

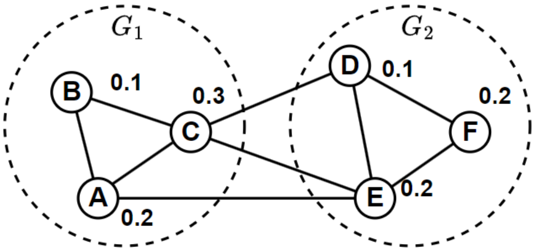


$$h_{N(i)}^{(k)} = \text{AGGREGATE}\left(\left\{h_u^{(k-1)}, \forall u \in N(i)\right\}\right)$$
$$h_i^{(k)} = \text{ReLU}\left(h_i^{(k-1)} \,||\, h_{N(i)}^{(k)}\right)$$

where || is a concatenation, $\text{ReLU}(x) = \max(0, x)$, *N(i)* is the neighbour nodes of node *i*.

   a) Calculate the feature of each node at $k = 1$.
   b) Calculate a graph-level embedding h_G by using a 'Mean' global pooling when $k = 1$.

2. Consider an undirected graph G of six nodes A, B, C, D, E and F given in the following figure. The graph G contains two cluster G_1 and G_2. Each node has initial features that are the numbers standing next to it. According to ClusterGCN model, the feature of a node i at layer k can be updated as:



$$h_{N(i)}^{(k)} = \text{MEAN}\left(\left\{h_u^{(k-1)}, \forall u \in N(i), G_u = G_i\right\}\right)$$
$$h_i^{(k)} = \text{ReLU}\left(h_i^{(k-1)} \,||\, h_{N(i)}^{(k)}\right)$$

where || is a concatenation.

Calculate the output representations of all nodes at layer $k = 1$.

3. Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

$$A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 2 \\ 1 \end{bmatrix}$$

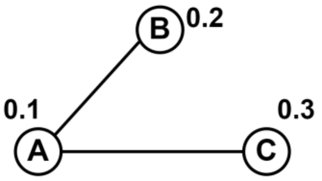
Assume that the output of an GCNII model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \sigma\left[\left((1-\beta)I_n\right) \cdot \left((1-\alpha)\tilde{A} \cdot H^{(k-1)} + \alpha H^{(0)}\right)\right]$$

where $H^{(k)}$ denotes the output at layer k, $\tilde{A}$ is the normalized matrix ($\tilde{A} = D^{-1}A$), I_n is the identity matrix, $\alpha = \beta = 0.5$, σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$.

   a) Calculate $\tilde{A}$.
   b) Calculate the output representations at layer $k = 1$.

4. Consider an undirected graph G of three nodes A, B, and C given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $h_A^{(0)} = 0.1$). According to GAT model, the weight matrix W is randomly initialized as [0.5]. The feature of node 'i' at layer (k) can be updated as:



$$h_i^{(k)} = \sigma\left(\sum_{m \in N(i)} \alpha_{im} W h_m\right)$$

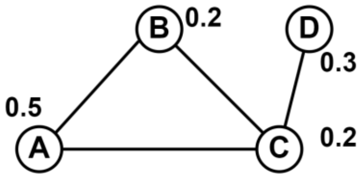
where: $\alpha_{im} = \frac{e_{im}}{\sum_{k \in N(i)} e_{ik}}$, and $e_{im} = \sigma\left(\mathrm{MEAN}\left(Wh_i, Wh_m\right)\right)$

σ is a ReLU function $\mathrm{ReLU}(x) = \max(0, x)$.

a) Calculate the attention coefficients e_{AB} and e_{AC}

b) Calculate the feature of node 'A' at $k = 1$.

5. Consider an undirected graph G of four nodes A, B, C, and D given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $h_A^{(0)} = 0.5$). According to GIN model, the parameter is a fixed scalar $\varepsilon = 0.5$, the feature of a node i at layer k can be updated as:

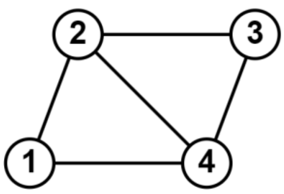


$$h_i^{(k)} = (1+\varepsilon) \cdot h_i^{(k-1)} + \sum_{j \in N(i)} h_j^{(k-1)}$$

a) Calculate the feature of each node at $k = 1$.

b) Calculate a graph-level embedding h_G by using a 'Max' global pooling when $k = 1$.

6. Consider an undirected graph G of four nodes given in the following figure. The Random Walk Positional Encoding, which is used in SAT model, of a node i can be calculated as:



$$p_i^{RWPE} = \left[\tilde{A}_{ii}, \tilde{A}_{ii}^2, \ldots, \tilde{A}_{ii}^k\right]$$

where $\tilde{A}$ is the normalized adjacency matrix $\tilde{A} = D^{-1}A$, $\tilde{A}^k$ is the k-step transition probability matrix $\tilde{A}^k = \underbrace{\tilde{A} \cdot \tilde{A} \cdots \tilde{A}}_{k}$. Calculate the positional encoding of each node at $k = 2$.